# 2017 Joint Nanoscience and Neutron Scattering User Meeting Poster Session

\*denotes Student Poster

Tuesday, August 1, 2017 5:30 – 7:00 p.m.

### Poster Location: Building 8600, Atrium

Posters will also be available for viewing on Wednesday, August 2

#### 01. A Computational Design Framework for Silicon Donor Qubits

Fahd A. Mohiyaddin<sup>1;2</sup>, Jacek Jakowski<sup>1;2;3</sup>, M. Nance Ericson<sup>1;4</sup>, Jingsong Huang<sup>1;2;3</sup>, Charles Britton<sup>1;5</sup>, Franklin G. Curtis<sup>1;2</sup>, Eugene F. Dumitrescu<sup>1;2;6</sup>, Bobby G. Sumpter<sup>1;2;3</sup>, and Travis S. Humble<sup>1;2;6</sup>

<sup>1</sup>Quantum Computing Institute, Oak Ridge National Laboratory, Oak Ridge, TN

#### 02. A Dichotomy in the Metastable-to-Ground State Vortex Lattice Transition in MgB<sub>2</sub>

E. R. Louden<sup>1</sup>, C. Rastovski<sup>1</sup>, L. DeBeer-Schmitt<sup>2</sup>, C. D. Dewhurst<sup>3</sup>, N. D. Zhigadlo<sup>4</sup>, J. Karpinski<sup>4</sup>, and M. R. Eskildsen<sup>1</sup>

<sup>1</sup>Department of Physics, University of Notre Dame, Notre Dame, Indiana 46656, USA

#### 03. Carbide-Phosphide Heterostructures for Electrochemical Water Splitting

Yagya N. Regmil<sup>1</sup>, Asa Roy<sup>2</sup>, Laurie A. King<sup>3</sup>, David. A. Cullen<sup>4</sup>, Harry M. Meyer III<sup>4</sup>, Gabriel A. Goenaga<sup>2</sup>, Thomas A. Zawodzinski Jr<sup>2</sup>, Nicole Labbé<sup>1</sup>, and Stephen C. Chmely<sup>1</sup>

<sup>1</sup>Center for Renewable Carbon, University of Tennessee, Knoxville, TN, 37996

#### 04. Characterization of the Interaction between Oxygen-Passivated Porous Graphene and Cations

Jonathan Heath and Marcelo A. Kuroda

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<sup>&</sup>lt;sup>4</sup>Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831, USA

### 05. Characterizing Poplar Molecular Structure using Chemical Imaging Techniques

E. Layden<sup>1</sup>, Songkil Kim<sup>2</sup>, U. Kalluri<sup>3</sup>, and O. Ovchinnikov<sup>2</sup>

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<sup>2</sup>Center for Nanophase Material Science, Oak Ridge National Laboratory, Oak Ridge, TN

<sup>3</sup>Plant Systems Biology, Oak Ridge National Laboratory, Oak Ridge, TN

#### 06. Colloidal assembly in nanochannel confinement

Roger Pynn<sup>1</sup>, Rana Ashkar<sup>2</sup>, Hao Feng<sup>1</sup>, Nickolay Lavrik<sup>2</sup>, Ivan Kravchenko<sup>2</sup>
<sup>1</sup>Indiana University, <sup>2</sup>Oak Ridge National Laboratory

#### 07. Colossal Bunching in Nanodiamond Cathodoluminescence

Matthew A. Feldman<sup>1,2</sup>, Roderick Davidson<sup>1,2</sup>, Jordan A. Hachtel<sup>1,2</sup>, Eugene F. Dumitrescu<sup>2</sup>, Raphael Pooser<sup>2</sup>, Anming Hu<sup>3</sup>, Denzel Bridges<sup>3</sup>, Phil Evans<sup>2</sup>, Richard F. Haglund<sup>1</sup>, Ben Lawrie<sup>2</sup> <sup>1</sup>Vanderbilt University, Department of Physics and Astronomy 6301 Stevenson Center Lane, Nashville, TN 37235-1807

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#### 08. Crystal structures of Ca-rich plagioclase feldspars with IT symmetry

Shiyun Jin\*, Xiaoping Wang \*\*, Huifang Xu \*

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\*\*Neutron Sciences Directorate, Oak Ridge National Laboratory, 1 Bethel Valley Road, Bldg. 8600, Mailstop 6475, Oak Ridge, TN 37831-6475, United States

#### 09. Curvature-Mediated Effects in Topographically Tunable Lipid Bilayers

Rana Ashkar<sup>1</sup>, Roger Pynn<sup>2</sup>, Nickolay Lavrik<sup>1</sup>, Ivan Kravchenko<sup>1</sup>, Jan-michael Carrillo<sup>1</sup>, Bobby Sumpter<sup>1</sup>, John Katsaras<sup>1</sup>

<sup>1</sup>Oak Ridge National Laboratory, <sup>2</sup>Indiana University,

# 10. Effects of magnetic fields on the dynamics in a single-molecule magnet. Quasi-elastic neutron scattering studies

Shelby E. Stavretis<sup>1</sup>, Duncan H. Moseley<sup>1</sup>, Eugene Mamontov<sup>2</sup>, Ziling Xue<sup>1</sup>

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<sup>2</sup>Chemical and Engineering Materials Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

#### 11. Enhanced Light-Matter Interaction and Optical Modulation with Silicon Photonics

F.O. Afzal, K. J. Miller, S. M. Weiss

Vanderbilt University

#### 12. Evaluating the diffusion and translocation of antibacterial treatment in plant systems

Nicholas Ciaffone<sup>1</sup>, Briana Lee<sup>1</sup>, Laurene Tetard<sup>1,2</sup>

<sup>1</sup>NanoScience Technology Center, University of Central Florida, Orlando, FL, 32826,

<sup>2</sup>Department of Physics, University of Central Florida, Orlando, Fl, 32816

### 13. Experimental and Computational Investigation of Microstructures and Mechanical Behavior of High-Entropy Alloys (HEAs)

P. K. Liaw<sup>1</sup>, H. Y. Diao<sup>1</sup>, T. K. Liu<sup>1</sup>, Y. F. Gao<sup>1</sup>, L. J. Santodonato<sup>1,2</sup>, Y. Zhang<sup>3</sup>, Jonathan Poplawsky<sup>2</sup>, Wei Guo<sup>2</sup>, M. Feygenson<sup>2</sup>, C. M. Parish<sup>2</sup>, M. C. Gao<sup>4,5</sup>, R. J. K. Weber<sup>6,7</sup>, J. C. Neuefeind<sup>2</sup>, Z. Tang<sup>1,8</sup>, Y. Zhang<sup>9</sup>, X. Xie<sup>1</sup>, S. Y. Chen<sup>1,9</sup>, T. T. Zuo<sup>1,9</sup>, Y. Zhu<sup>1</sup>, S. Kuo<sup>2</sup>, M. Widom<sup>10</sup>, D. J. Keffer<sup>1</sup>, K. An<sup>2</sup>, D. Ma<sup>2</sup>, A. Stoica<sup>2</sup>, T. Egami<sup>1,2</sup>, J. R. Morris<sup>1,2</sup>, L. Collins<sup>2</sup>, J. W. Yeh<sup>11</sup>, C. W. Tsai<sup>11</sup>, R. R. Unocic<sup>2</sup>, K. Littrell<sup>2</sup>, and K. A. Dahmen<sup>12</sup>

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<sup>12</sup>Dept. of Physics, University of Illinois at Urbana Champaign, USA

### 14. High volume sampling and data analysis for nanoscience: building an open-source toolkit for CNMS

P. Doak and P. Ganesh

Center for Nanophase Material Science, Oak Ridge National Laboratory

### **15.** Impact of surface interaction on charge transport in ultra-thin films of polymerized ionic liquids Maximilian Heres, Tyler Cosby, Joshua Sangoro

University of Tennessee, Knoxville, TN 37920

### 16. In Situ Dilatometry of Electrochemical Proton Intercalation into Hydrated and Anhydrous Tungsten Oxides

Ruocun (John) Wang<sup>1</sup>, James B. Mitchell<sup>1</sup>, Qiang Gao<sup>2</sup>, Wan-Yu Tsai<sup>2</sup>, Nina Balke<sup>2</sup>, Veronica Augustyn<sup>1</sup>

<sup>1</sup>Department of Materials Science and Engineering, North Carolina State University, NC 27695

<sup>2</sup>Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6496

#### 17. Influence of Mesoscale Organization on Charge Transport and Dynamics in Ionic Liquids

Tyler Cosby<sup>1</sup>, Zachariah Vicars<sup>1</sup>, Yangyang Wang<sup>2</sup>, and Joshua Sangoro<sup>1</sup>

<sup>1</sup>University of Tennessee, Department of Chemical and Biomolecular Engineering, Knoxville, TN 37902

<sup>2</sup>Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN 37831

### 18. Ion Beam Induced Current - Stage Design and Experiment

R. Cannon Buechley, Olga Ovchinnikova, Matthew Burch, Songkil Kim, Stephen Jesse, Alex Belianinov

The Center for Nanophase Material Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831

#### 19. Linking the Mechanisms of Na-Ion Binding to the Structure of Amorphous Hard Carbon

T. W. Surta<sup>a</sup>, Z. Lia, C. Bommier<sup>a</sup>, X. Ji<sup>a</sup>, P. A. Greaney<sup>b</sup>, M. R. Dolgos<sup>a</sup>

<sup>a</sup>Oregon State University, Corvallis, OR 97330

<sup>b</sup>University of California Riverside, Riverside, CA 92521

#### 20. Measurement and Modeling of Structure and Dynamics in Doped Organic Semiconductors

Adam Moule, Tucker Murrey, Ian Jacobs, Jun Li, Thomas Harrelson University of California, Davis

#### 21. Metallic Neutron Guides by Replication Superpolished Glass or Metal Mandrels

Boris Khaykovich<sup>1</sup>, Darrell Engelhaupt<sup>2</sup>, Suzanne Romaine<sup>3</sup>, Mikhail Gubarev<sup>4</sup>

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<sup>2</sup>Smithsonian Astrophysical Observatory, Cambridge, MA 02138, USA

<sup>3</sup>Marshall Space Flight Center, NASA, Huntsville, AL 35812, USA

#### 22. Microstructural Characterization on Novel Creep-Resistant Ferritic Superalloys

Shao-Yu Wang<sup>1</sup>, Zongyang Lyu<sup>1</sup>, David C. Dunand<sup>2</sup>, Gautam Ghosh<sup>2</sup>, Sungil Baik<sup>2</sup>, Peter K. Liaw<sup>1</sup> Department of Materials Science and Engineering, The University of Tennessee (UT), Knoxville, TN 37996, USA

<sup>2</sup>Department of Materials Science and Engineering, Northwestern University (NU), Evanston, IL 60208-3108, USA

#### 23. Neutron vibrational spectroscopy and surface chemistry: catalysts and porous materials

A.J. Ramirez-Cuesta, Y.Q. Cheng, A. Sharma, Z. Wu, D.A. Lutterman, M. Kidder, S. Tan, A.A. Savara, L.L. Daemen

Oak Ridge National Laboratory, Oak Ridge, TN

### 24. One-step Synthesis of Nb2O5/C/Nb2C (MXene) Composites and Their Use as Photocatalysts for Hydrogen Evolution

Tongming Su<sup>a,b,c</sup>, Rui Peng<sup>b</sup>, Zachary D. Hood<sup>b,e</sup>, Michael Naguib<sup>d</sup>, Ilia N. Ivanov<sup>b</sup>, Jong Kahk Keum<sup>b</sup>, Zuzeng Qin<sup>a,\*</sup>, Zhanhu Guo<sup>c,\*</sup>, and Zili Wu<sup>b,\*</sup>

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#### 25. Phase Stability and Transformation in a Light-weight High-entropy Alloy

Rui Feng<sup>1</sup>, Michael C. Gao<sup>2,3,\*</sup>, Chuan Zhang<sup>4</sup>, Wei Guo<sup>5</sup>, Jonathan D. Poplawsky<sup>5</sup>, Fan Zhang<sup>4</sup>, Jeffrey A. Hawk<sup>2</sup>, Joerg C. Neuefeind<sup>6</sup>, Yang Ren<sup>7</sup>, and Peter. K. Liaw<sup>1,\*</sup>

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### 26. Phosphonium-Containing Block Copolymers from Living Anionic Polymerization of 4-Diphenylphosphino Styrene

Philip J. Scott<sup>a</sup>, Alison R. Schultz<sup>a</sup>, Gregory B. Fahs<sup>a</sup>, Chainika Jangu<sup>a</sup>, Mingtao Chen<sup>a</sup>, Robert B. Moore<sup>a</sup>, David Uhrig<sup>b</sup>, Bradley S. Lokitz<sup>b</sup>, and Timothy E. Long<sup>a</sup>

<sup>a</sup>Department of Chemistry, Macromolecules Innovation Institute (MII), Virginia Tech

<sup>b</sup>Center for Nanophase Materials Sciences Division, Oak Ridge National Laboratory

# 27. Photoinduced Thermal Desorption Coupled with Atmospheric Pressure Chemical Ionization Mass Spectrometry for Multimodal Imaging

Matthias Lorenz<sup>1</sup>, Chance Brown<sup>1</sup>, Roger Proksch<sup>2</sup>, Mario Viani<sup>2</sup>, Aleks Labuda<sup>2</sup>, Stephen Jesse<sup>3</sup>, and Olga Ovchinnikova<sup>3</sup>

<sup>1</sup>University of Tennessee, Knoxville; <sup>2</sup>Oxford Instruments; <sup>3</sup>Oak Ridge National Laboratory

### 28. Polymers Undergoing Pairwise Head-to-Head Association and Dissociation: Molecular Dynamics Model, Reaction Kinetics, and Linear Viscoelastic Relaxation

Wen-Sheng Xu<sup>1</sup>, Jan-Michael Y. Carrillo<sup>1,2</sup>, and Yangyang Wang<sup>1</sup>

<sup>1</sup>Center for Nanophase Materials Sciences and <sup>2</sup>Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, United States

#### 29. Radiation-Induced Correlated Disorder and its Impact on Ionic Conductivity

Eric O'Quinn<sup>1</sup>, Jacob Shamblin1;2, Joerg Neuefeind3, Maik Lang1

<sup>1</sup>Department of Nuclear Engineering, University of Tennessee, TN, 37996, USA

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<sup>3</sup>Chemical and Engineering Materials Division, Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831

# 30. Rapid Screening of Nanoporous Structures in SiO-2 Catalyst Particles via Helium Ion Microscopy

Matthew J. Burch<sup>1</sup>, Anton V. Ievlev<sup>1</sup>, Holland Hysmith<sup>1</sup>, Kyle Mahady<sup>2</sup>, Philip D. Rack<sup>1,2</sup>, Lubin Luo<sup>3</sup>, Alex Belianinov<sup>1</sup>, Sergey Yakovlev<sup>3</sup>, and Olga S. Ovchinnikova<sup>1\*</sup>.

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<sup>3</sup> Global Product Research, ExxonMobil Chemical Company, Baytown, TX 77520, USA

### 31 Role of dipolar interactions on Flory-Huggins chi parameter

Dr. KUMAR, Rajeey; Dr. SUMPTER, Bobby

J. P. Mahalik, Bobby Sumpter, and Rajeev Kumar

Center for Nanophase Materials Science, Oak Ridge National Laboratory, Oak Ridge, TN

### 32 SANS Investigation of Multiple Stage Self Assembly of Polythiophene Supramolecular Structures Prepared by Ex Situ Initiated Controlled Chain-Growth Polymerization

C.P. Kei, C. Do and E.E. Nesterov

Department of Chemistry, Louisiana State University, Baton Rouge, LA 70803 Spallation Neutron Source, Oak Ridge National Laboratory, Oak Ridge, TN 37831

#### 33 Soft Nanostructures for Energy Storage

Jihua Chen

#### 34 STEM and HIM Investigations of Carbon Nanostructures in Copper Covetic Materials

Beihai Ma<sup>1</sup>, Uthamalingam Balachandran<sup>1</sup>, Jianguo Wen<sup>2</sup>, Jie Wang<sup>2</sup>, and Adam J. Rondinone<sup>3</sup>
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#### 35 Structural and electronic complexity in a model cathode material NaMnO2

Rebecca Dally and Stephen D. Wilson

Materials Department, University of California, Santa Barbara, Santa Barbara, California 93427

#### 36 Structural disorder study of Ce(Rh,T) across the ferromagnetic phase transition

Jean-Guy Lussier<sup>1</sup>, Adane Gebretsadik<sup>1</sup>, Almut Schroeder<sup>1</sup>, Katharine Page<sup>2</sup>

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### 37 Synthesis and Characterization of New High Temperature Multigraft Copolymer Superelastomer: Polyisoprene-graft-polybenzofulvene

Huiqun Wang, Weiyu Wang, Wei Lu, Nam-Goo Kang\*, Jimmy Mays\* Department of Chemistry, University of Tennessee, Knoxville, TN 37996

### 38 Understanding and Controlling Dynamics of Graphene Milling Process Using Helium Ion Beam

Songkil Kim<sup>1,2</sup>, Anton V. Ievlev<sup>1,2</sup>, Ivan V. Vlassiouk<sup>3</sup>, Matthew J. Burch<sup>1,2</sup>, Ondrej E. Dyck<sup>1,2</sup>, Xiahan Sang<sup>1,2</sup>, Raymond R. Unocic<sup>1,2</sup>, Alex Belianinov<sup>1,2</sup>, Sergei V. Kalinin<sup>1,2</sup>, Stephen Jesse<sup>1,2</sup> and Olga S. Ovchinnikova<sup>1,2</sup>

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#### 39 Unique Capabilities for Neutron Investigations of Surface and Materials Chemistry

Christopher Crain, Daniele Paradiso, Nicholas Strange, Fatema Wahida, J.Z. Larese Department of Chemistry, University of Tennessee, Knoxville

#### 40 Waste-to-Biofuel Conversion Using Carbon-Based Acid Catalysts Derived from Recycled Tires

S. P. Adhikari<sup>1,2</sup>, Z. D. Hood<sup>3,4</sup>, M. Wright<sup>1</sup>, M. P. Paranthaman, <sup>5,6</sup> and A. Lachgar<sup>1,2</sup>

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### 41\* Ab Initio Explorations of a New Class of Quaternary ZrBCN Nanocomposite Coatings for Harsh Environments

Chongze Hu<sup>1</sup>, Jingsong Huang<sup>2</sup>, Bobby G. Sumpter<sup>2</sup>, Jiechao Jiang<sup>3</sup>, Efstathios Meletis<sup>3</sup>, and Traian Dumitrica<sup>1</sup>

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#### 42\* All Acrylic Mulitigraft Copolymer Superelastomer

Wei Lu<sup>1</sup>, Andrew Goodwin<sup>1</sup>, Yangyang Wang<sup>2</sup>, Weiyu Wang<sup>2</sup>, Panchao Yin<sup>2</sup>, Xinyi Lu<sup>1</sup>, Kunlun Hong<sup>2</sup>, Nam-Goo Kang<sup>1</sup>, Jimmy Mays<sup>1</sup>

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#### 43\* Centrifugal-driven, reduced-dimension, planar chromatography

Rachel Strickhouser<sup>1</sup>, Nahla Hatab<sup>1</sup>, Nickolay Lavrik<sup>2</sup>, Michael Sepaniak<sup>1</sup>

<sup>1</sup>University of Tennessee

<sup>2</sup>Center of Nanophase Materials Sciences

### 44\* Exploring Ferroelectric/Ferromagnetic Interactions Created by Hybrid Organic-Inorganic Perovskites and Nickel

Yongtao Liu, Kai Xiao, Scott T. Retterer, Bin Hu, Olga S. Ovchinnikova Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN Department of Materials Science and Engineering, University of Tennessee, Knoxville, TN

# 45\* Inverse Estimation of Surface Fractal Dimension and Aperture Width for Rock Fractures Imaged with Neutron Radiography

J.W. Brabazon<sup>a</sup>, E. Perfect<sup>a</sup>, C.-L. Cheng<sup>b</sup>, H.Z. Bilheux<sup>c</sup>, A.S. Tremsin<sup>d</sup>, and L.J. Santodonato<sup>e</sup>

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# 46\* Investigation on crystal structure of deuterated schwertmannite using Z-contrast images and neutron pair distribution function analysis

Seungyeol Lee and Huifang Xu

Department of Geoscience, University of Wisconsin – Madison

# 47\* Microstructural Evolution and Mechanical Behavior of NbTaTiV Refractory High-entropy Alloy at Elevated Temperatures

Chanho Lee<sup>1</sup>, Gian Song<sup>2</sup>, Michael C. Gao<sup>3</sup>, Chuan Zhang<sup>4</sup>, Rui Feng<sup>1</sup>, Peiyong Chen<sup>1</sup>, Yan Chen<sup>5</sup>, Ke An<sup>5</sup>, Wei Guo<sup>6</sup>, Jonathan Poplawsky<sup>6</sup>, Choo Hahn<sup>1</sup>, and Peter K. Liaw<sup>1\*</sup>

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#### 48\* Nanoscale functional characterization of 2D materials

Chance Barrett<sup>a,b</sup>, Yi Ding<sup>b,c</sup>, Laurene Tetard<sup>a,b,c</sup>

<sup>a</sup>Physics Department, <sup>b</sup>NanoScience Technology Center, <sup>c</sup>Materials Science and Engineering Department, University of Central Florida, Orlando, FL

# 49\* Nanoscale investigation of biophysicochemical responses to multivalent nanoparticle treatment on Xanthomonas perforans

Briana Lee<sup>1</sup>, Ali Ozcan<sup>2</sup>, Swadeshmukul Santra<sup>1,2</sup>, Laurene Tetard<sup>1,3</sup>

<sup>1</sup>NanoScience Technology Center, University of Central Florida, Orlando, FL, 32826,

### 50\* Ni/Al-Based Reactive Multilayer Films for Low Temperature Brazing in Microgravity Environments

D. Bridges<sup>1</sup>, C.M. Rouleau<sup>2</sup>, D.B. Geohegan<sup>2</sup>, Y. Bar-Cohen<sup>3</sup>, A. Hu<sup>1</sup>

<sup>1</sup>Department of Mechanical, Aerospace, and Biomedical Engineering, University of Tennessee, Knoxville

### 51\* Palladium diselenide, a new 2D semiconductor with tunable bandgaps and high mobility for electronics

Akinola Oyedele<sup>1,2</sup>, Shize Yang<sup>3</sup>, Liangbo Liang<sup>2</sup>, Alexander A Puretzky<sup>2</sup>, Chris Rouleau<sup>2</sup>, Bobby G. Sumpter<sup>2</sup>, David B. Geohegan<sup>2</sup>, Kai Xiao<sup>2,1\*</sup>

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# 52\* Photoinduced Bulk Polarization in Perovskite Solar Cells via Photoinduced Impedance and Kelvin-Probe Force Microscopy Study

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#### 53\* Physical properties of the cubic spinel LiGaCr4S8

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#### 54\* Stress Effect on Electronic and Thermoelectric Properties of Skutterudite

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### 55\* Synthesis and characterization of defect-laden h-BN for applications in heterogeneous catalytic reactions

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### 56\* Tailoring Thermomechanical and Actuation Properties of Liquid Crystalline Elastomers

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### 57\* TOF-SIMS Investigation of Tip-Surface Chemical Interactions in Atomic Force Microscopy on a Combined AFM/ToF-SIMS Platform

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### 58\* Tracking the Uptake and Translocation of Zinc-based Treatments Designed to Combat Citrus Greening Disease

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### 59\* Two-dimensional Jeff = 1/2 antiferromagnetic insulator unraveled from interlayer exchange coupling in artificial perovskite iridate superlattices

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# 60\* Understanding Nano-scale Electro-response: Ionic Liquid Containing Diblock Copolymers Synthesis

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### 61\* Yb2Si2O7 Understanding Magnetic Correlations in a Novel Honeycomb Structure

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